

**This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U. S. Department of Energy.**

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## Appendix E - First-order mass transfer coefficient estimation assuming pure diffusion

Consider purely diffusive mass transfer to the immobile region from a surrounding, constant concentration, mobile region. This one-dimensional, transient, mass diffusion problem can be stated as

$$\begin{aligned}\frac{\partial^2 C}{\partial x^2} &= \frac{1}{D^*} \frac{\partial C}{\partial t} \\ C(0,t) &= C(L,t) = C_\infty \\ C(x,0) &= C_i\end{aligned}\tag{1}$$

The problem can be made non-dimensional by defining

$$\begin{aligned}\xi &= x/L \\ \tau &= D^* t / L^2 \\ u &= \frac{C - C_\infty}{C_i - C_\infty}\end{aligned}\tag{2}$$

and equations (1) become

$$\begin{aligned}u_{xx} &= u_\tau \\ u(0,t) &= 0 \\ u(x,0) &= 1\end{aligned}\tag{3}$$

By analogy to plane-wall transient heat conduction (Myers, 1971, section 3.1.1), the analytical solution is (Myers, 1971, equation (3.1.7))

$$u(\xi, \tau) = 4 \sum_{m=0}^{\infty} \frac{\sin \beta_m \xi}{\beta_m} e^{-\beta_m^2 \tau}\tag{4}$$

where

$$\beta_m = (2m+1)\pi\tag{5}$$

The dimensional concentration becomes

$$C = C_\infty + u(C_i - C_\infty)\tag{6}$$

Under the current nomenclature, the dual-media mass transfer coefficient would be defined by

$$\theta_{im} \frac{\partial \bar{C}}{\partial t} = \beta(C_{\infty} - \bar{C}) \quad (7)$$

where

$$\bar{C} = \frac{\int_0^L C \theta_{im} dx}{\theta_{im} L} = \frac{1}{L} \int_0^L C dx \quad (8)$$

Substituting (6) produces

$$\begin{aligned} \bar{C} &= \frac{1}{L} \int_0^L C dx \\ &= \frac{1}{L} \int_0^L [C_{\infty} + u(C_i - C_{\infty})] dx \\ &= C_{\infty} + (C_i - C_{\infty}) \frac{1}{L} \int_0^L u dx \\ &= C_{\infty} + (C_i - C_{\infty}) \int_0^L u d(x/L) \\ &= C_{\infty} + (C_i - C_{\infty}) \int_0^1 u d\xi \end{aligned} \quad (9)$$

or in non-dimensional form

$$\frac{\bar{C} - C_{\infty}}{C_i - C_{\infty}} = \bar{u} = \int_0^1 u d\xi \quad (10)$$

From equation (4) the integral is evaluated as

$$\begin{aligned}
\bar{u} &= \int_0^1 4 \sum_{m=0}^{\infty} \frac{\sin \beta_m \xi}{\beta_m} e^{-\beta_m^2 \tau} d\xi \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \int_0^1 \sin \beta_m \xi d\xi \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \left[ \frac{-\cos \beta_m \xi}{\beta_m} \right]_0^1 \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \frac{1}{\beta_m} [-\cos \beta_m + 1] \\
&= 4 \sum_{m=0}^{\infty} \frac{1}{\beta_m} e^{-\beta_m^2 \tau} \cdot \frac{1}{\beta_m} [1 + 1] \\
&= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m^2} e^{-\beta_m^2 \tau}
\end{aligned} \tag{11}$$

Equation (7) can be written in a non-dimensional form as

$$\begin{aligned}
\theta_{im} \frac{\partial \bar{C}}{\partial t} &= \beta (C_{\infty} - \bar{C}) \\
\frac{\partial \bar{C}}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_{\infty}) \\
\frac{\partial (\bar{C} - C_{\infty})}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_{\infty}) \\
\frac{\partial (\bar{C} - C_{\infty}) / (C_i - C_{\infty})}{\partial t} &= -\frac{\beta}{\theta_{im}} (\bar{C} - C_{\infty}) / (C_i - C_{\infty}) \\
\frac{\partial \bar{u}}{\partial t} &= -\frac{\beta}{\theta_{im}} \bar{u} \\
\frac{\partial \bar{u}}{\partial (\tau L^2 / D^*)} &= -\frac{\beta}{\theta_{im}} \bar{u} \\
\frac{\partial \bar{u}}{\partial \tau} &= -\frac{\beta L^2}{\theta_{im} D^*} \bar{u}
\end{aligned} \tag{12}$$

Solving for the mass transfer coefficient yields

$$\beta = \frac{\theta_{im} D^*}{L^2 \bar{u}} \left( -\frac{\partial \bar{u}}{\partial \tau} \right) \tag{13}$$

The time derivative is computed as

$$\begin{aligned}
 \frac{\partial \bar{u}}{\partial \tau} &= \frac{\partial}{\partial \tau} \left[ 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m^2} e^{-\beta_m^2 \tau} \right] \\
 &= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m^2} \cdot \frac{\partial}{\partial \tau} e^{-\beta_m^2 \tau} \\
 &= 8 \sum_{m=0}^{\infty} \frac{1}{\beta_m^2} \cdot \left( -\beta_m^2 e^{-\beta_m^2 \tau} \right) \\
 &= -8 \sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}
 \end{aligned} \tag{11}$$

or

$$-\frac{\partial \bar{u}}{\partial \tau} = 8 \sum_{m=0}^{\infty} e^{-\beta_m^2 \tau} \tag{12}$$

The dual-media mass transfer coefficient becomes

$$\begin{aligned}
 \beta &= \frac{\theta_{im} D^*}{L^2} \cdot \frac{-\frac{\partial \bar{u}}{\partial \tau}}{\bar{u}} \\
 &= \frac{\theta_{im} D^*}{L^2} \cdot \frac{8 \sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}}{8 \sum_{m=0}^{\infty} \frac{1}{\beta_m^2} e^{-\beta_m^2 \tau}} \\
 &= \frac{\theta_{im} D^*}{L^2} \cdot \frac{\sum_{m=0}^{\infty} e^{-\beta_m^2 \tau}}{\sum_{m=0}^{\infty} \frac{1}{\beta_m^2} e^{-\beta_m^2 \tau}}
 \end{aligned} \tag{13}$$

## References

Myers, G. E., 1971, Analytical methods of conduction heat transfer, McGraw-Hill, New York.